# DIFFICULTY AND POSSIBILITY OF KINETIC THEORY OF QUANTUM-MECHANICAL SYSTEMS

## Part V — Particular and General Solutions of the Schrodinger Equation and their Significance in Kinetic Theory

by

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## SUMMARY

The quantum-mechanical Liouville equation is more restrictive and hence more informative than the Schrodinger equation, because the former already contains the definition of independent variable $\vec{p}$, momentum in a special case. In this sense, the quantum-mechanical Liouville equation is more definitive as the description of a physical law, and is shown to be invariant under the Galilean transformation. By taking advantage of this convenience, we obtain a particular solution of the Schrodinger equation for n-particle system. This solution is localized in the phase space and stable in time, and seems to represent an n-particle system as single system. The de Broglie wave is constructed by superposing a number of similar particular solutions for single-particle systems. Similarly, general solution is constructed for n-particle systems. For justification of its application to kinetic theory, Pauli's principle is analyzed and interpreted anew. The present solution promises the possibility of rational methods of kinetic theory of quantum-mechanical systems, as analogous to methods of classical kinetic theory.

## I. INTRODUCTION

In this report, it will be shown that the Schrodinger equation for n-particle system has an exact solution which appears in various aspects to represent a single system, and that the solution is significant in kinetic theory.

The essential part of the orthodox quantum mechanics consists of the definitions of observables, measurements and representations of systems, and commutation relations and dynamical laws governing observables. Consideration of the Schrodinger equation or the Dirac equation is merely an auxiliary or subsidiary matter.

On the other hand, there are some authors (Ref. 1) who state, sometimes tacitly, that the Schrodinger equation or the Dirac equation are basic laws; when we choose a certain family of their solutions, major axioms of the orthodox quantum mechanics turn out mere theorems.* In a previous report (Ref. 2), a similar anomalous view was advanced, and it was demonstrated that the view is rational and furthermore is necessary for treating a system in its evolution. According to this view, conventional eigen solutions of the Schrodinger equation are of ensembles,

*This might remind one that Heaviside's operator rules turned out theorems, when basic differential equations of electromagnetic phenomena were solved by methods of Fourier transformation and of Laplace transformation. Here, certainly, Schrodinger himself should be mentioned.

instead of single systems, and hence are useless for the basis of treating a system in its evolution in the kinetic theoretical sense. If this be true in general, those Hamiltonian observables of electron-electron and electron-photon interactions may contain some inconsistencies, because they are constructed from the plane wave representation of electron which we regard as of ensemble (Ref.2). Indeed, inconsistencies were shown to exist, as expected, in those Hamiltonians in another report (Ref.3).

Thus far, however, alternate representations of single systems have not been proposed. Sometimes a wave packet is thought to be the one for single particle. But a conventional wave packet does not satisfy exactly the Schrodinger equation and hence is not stable. In this report, we shall show that the quantum-mechanical Liouville equation derived in Ref.2 leads to discovery of a stable wavelet which satisfies exactly the Schrodinger equation. Construction of ensemble representations of similar wavelets is also made.

However, it should be remarked in advance that the present wavelet is made as spherically symmetric. In general this condition is too restrictive that ensemble solutions constructed with the present wavelet solutions do not result in eigenfunctions particularly for some lowest energy levels. This situation is easily predictable, since a wavelet is most unlikely to be

spherically symmetric in a potential field of steep gradient. Nevertheless, the wavelet is an exact solution of the Schrodinger equation, regardless of the field. This seems to imply that its deformation in a force field be designed rather easily.

For treating an n-particle system in classical kinetic theory, we begin with a particular solution of the Louville equation; the solution is represented in terms of $\delta$-functions:

$$D = \prod_{k=1}^{n} \delta(\vec{r}_k - \vec{r}_k(t)) \, \delta(\vec{p}_k - \vec{p}_k(t)) \tag{1.1}$$

Here $\delta(\vec{r}_k - \vec{r}_k(t)) = \delta(x_k - x_k(t)) \, \delta(y_k - y_k(t)) \, \delta(z_k - z_k(t))$, etc., $\vec{r}_k(t)$, $\vec{p}_k(t)$ are solutions of Newton's equations

$$\begin{aligned} &m_k \dot{\vec{r}}_k(t) = \vec{p}_k(t) \\ &\dot{\vec{p}}_k(t) = -\,\mathrm{grad}_k U \\ &U: \text{potential.} \qquad (k = 1, 2, \ldots, n) \end{aligned} \tag{1.2}$$

and $\vec{r}_k$, $\vec{p}_k$ are independent variables. Of course, we cannot solve Eqs.(1.2) for more than two particles. Nevertheless, solution (1. 1) provides a restriction necessary for the proper treatment of a system in the kinetic-theoretical sense. Ref. 4.

In this report, we shall show that the Schrodinger equation for n particles has a solution similar to, but not the same as, Eq.(1.1). Furthermore, those functions of t, $\vec{r}_k(t)$, $\vec{p}_k(t)$, etc. are governed by the same set of equations as Eqs.(1.2). This

is a remarkable convenience, particularly for kinetic theory.

In section II, we discuss the invariance of the quantum-mechanical Liouville equation under the Galilean transformation. The invariance provides a clue for solving the Schrodinger equation which is not invariant under the same transformation. In section III, we first get a solution of the quantum-mechanical Liouville equation which is time-independent and localized in space. By means of the Galilean transformation, we then get the representation of the same solution given with respect to a coordinate system moving uniformly relative to the initial system. This solution is neither energy eigenfunction nor momentum eigenfunction in the conventional sense. Nevertheless, it represents characteristics of particle. Furthermore, it is possible to construct a de Broglie wave by superposing many similar solutions obtained by merely changing the phase in the solution. In section IV, we derive the quantum-mechanical Liouville equation for n-particle systems. Based on this, in section V, we discuss the meaning of Pauli's principle. This is done for making the conclusion reached in section III as compatible with the conventional interpretation of eigen-solutions of the Schrodinger equation. In the light of these findings, we obtain in section VI a particular solution of the Schrodinger equation for n-particle system. The solution is remarkably similar to (1.1); yet it retains all the characteristics proper to quantum-mechanical particles. Its significance is discussed in sections VII and VIII.

## II. INVARIANCE UNDER THE GALILEAN TRANSFORMATION

Dynamical variables of a particle observed by an observer fixed to a coordinate system, one of the inertial systems, are given by

$\vec{r}'$ : position vector,

$\vec{p}'$ : momentum.

We consider another observer fixed to the second coordinate system which moves with a constant velocity $-\vec{v}$ relative to the first system. Dynamical variables of the same particle observed by the second observer are

$\vec{r}$ : position vector

$\vec{p}$ : momentum

and

$$\vec{r} = \vec{r}' + \vec{v}t, \tag{2.1}$$

$$\vec{p} = \vec{p}' + m\vec{v}. \tag{2.2}$$

Newton's equations of motion are invariant under the Galilean transformation of variables according to (2.1) and (2.2), if $\vec{v}$ is invariant. The classical Liouville equation is also invariant under the same transformation. This is readily shown by that, with respect to a function f of $\vec{r}'$, $\vec{p}'$, t

$$f(\vec{r}', \vec{p}', t) \equiv f(\vec{r}-\vec{v}t, \vec{p}-m\vec{v}, t)$$

$$(\partial f/\partial t)_{r',p'} = (\partial f/\partial t)_{r,p} + \vec{v}\cdot(\partial f/\partial \vec{r})_{t,p}$$

$$(\partial f/\partial \vec{r}')_{t,p'} = (\partial f/\partial \vec{r})_{t,p} \qquad (2.3)$$

etc.

On the other hand, the Hamilton-Jacobi equation and also the Schrodinger equation are not invariant under the Galilean transformation. From the mathematical viewpoint , this is because these equations are linear with respect to operator $\partial/\partial t$, and nonlinear with respect to $\partial/\partial \vec{r}$. From the physical viewpoint, the Hamilton-Jacobi equation alone cannot represent the complete set of dynamical laws; it needs the definition of momentum as an independent vector variable for being complete. With the definition of momentum, the equation is reduced to the Liouville equation which is complete as a representation of Newton's dynamical law. (The initial Hamilton-Jacobi equation is then the expression of energy conservation.) In a similar manner, the Schrodinger equation alone is not a complete physical law; it needs the physical definitions of momentum and energy.

Previously, Ref.2, we derived the quantum-mechanical Liouville equation from the Schrodinger equation. In the process of derivation, we defined an independent vector variable $\vec{p}$. Thus the quantum-mechanical Liouville equation is more restrictive and more informative than the Schrodinger equation alone, in the

same way as the classical Liouville equation is more restrictive and more informative than the Hamilton-Jacobi equation alone. As a result, the quantum-mechanical Liouville equation is invariant under the Galilean transformation, provided that $\vec{p}$ is transformed according to (2.2). The last condition is a new assumption or interpretation which has not been made with respect to the Schrodinger equation. This is justified as follows:

For the convenience of reference, we write here some results obtained in Part II of this report (Ref.2): We saw that the Schrodinger equation for single particle leads to

$$\psi = a \exp(iS/\hbar) \tag{2.4}$$

$$\partial S/\partial t + p^2/2m + U - (\hbar^2/2m)(\Delta a/a) = 0 \tag{2.5}$$

$$\left[\frac{\partial}{\partial t} + \frac{p}{m}\cdot\text{grad} - \text{grad}\left(U - \frac{\hbar^2}{2m}\frac{\Delta a}{a}\right)\right] a^2 = 0 \tag{2.6}$$

on the definition

$$\vec{p} = \text{grad } S \tag{2.7}$$

Equation (2.6) is what we call the quantum-mechanical Liouville equation. There, also we saw that the energy eigen-function leads to the energy eigen-value

$$E = U + p^2/2m - (\hbar^2/2m)(\Delta a/a) \tag{2.8}$$

(Eq.(4.4)' in Ref.2)

and, if $\Delta a/a$ is moderate, the quantum-mechanical Liouville

equation (2.6) has characteristic equations

$$\frac{d\vec{p}}{dt} = -\text{grad } U + \frac{\hbar^2}{2m} \text{grad}\left(\frac{\Delta a}{a}\right) \tag{2.9}$$

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} \tag{2.10}$$

Obviously, (2.8) is the integral of (2.9) under condition (2.10); and (2.10) implies (2.2).

## III. A PARTICULAR SOLUTION OF THE SCHRODINGER EQUATION

Helped by the Galilean invariance principle, we obtain an interesting solution of the Schrodinger equation for single particle. We first suppose that there is a solution $a^2$ of Eq.(2.6) under the condition that

$$\partial a^2/\partial t = 0, \quad \vec{p} = 0, \text{ grad } U = 0 \tag{3.1}$$

Then Eq.(2.6) yields

$$\text{grad}(\Delta a/a) = 0, \text{ or } \Delta a/a = \text{const} = K \tag{3.2}$$

A well-known solution of (3.2) is

$$a = \exp(-K^{1/2} r)/r \tag{3.3}$$

$$(r^2 = x^2 + y^2 + z^2)$$

Since a should be real, K should be positive:

$$K = \kappa^2 > 0 \tag{3.2}'$$

If we take another coordinate system which is moving uniformly with $-\vec{v}$ relative to the initial one, we have to substitute for $\vec{r}$

$$\vec{r} - \vec{v}t \tag{3.4}$$

and

$$\vec{p} = m\vec{v} \tag{3.5}$$

according to (2.2). Hence (3.3) yields

$$a^2 = \frac{\exp(-2\kappa|\vec{r} - \vec{v}t|)}{|\vec{r} - \vec{v}t|^2} \tag{3.6}$$

which is a solution of (2.6) when grad U = 0. In accordance with (3.5), we take for S

$$S = -Et + m\vec{v}\cdot\vec{r} \tag{3.7}$$

which satisfies Eq.(2.5) under the condition

$$E = mv^2/2 - \hbar^2\kappa^2/(2m) \tag{3.8}$$

Since $\vec{v}$ and $\kappa$ are invariant, E is also an invariant. Finally,

$$\psi = \frac{\exp(-\kappa|\vec{r} - \vec{v}t|)}{|\vec{r}-\vec{v}t|} \exp\left[i(-Et + m\vec{v}\cdot\vec{r})/\hbar\right] \tag{3.9}$$

is a solution of the Schrodinger equation under condition (3.8).

We now intend to find a solution when

$$\text{grad } U \neq 0$$

In this case, in general, there is no definite justification of (3.2). But we assume that

a) grad U is weak so that (3.2) is valid to an approximation; or

b) there is another additional condition which justifies (3.2).

Then it is easy to write down the result by modifying (3.9):

$$a = \frac{\exp\left[-\kappa/(r - \int \frac{\vec{p}(t)}{m} dt)\right]}{\left|\vec{r} - \int \frac{\vec{p}(t)}{m}\, dt\right|} \delta^{1/2}(\vec{p} - \vec{p}(t)) \qquad (3.10)$$

where *

$$\left[\delta^{\frac{1}{2}}(\vec{p} - \vec{p}(t)\right]^2 \equiv \delta(\vec{p} - \vec{p}(t))$$
$$\equiv \delta(p_x - p_x(t))\,\delta(p_y - p_y(t))\,\delta(p_z - p_z(t))$$

and $\vec{p}(t)$ satisfies Eqs.(2.9) and (2.10), under condition (3.2).

$$d\vec{p}/dt = -\text{grad } U, \quad d\vec{r}/dt = \vec{p}/m \qquad (3.11)$$

Finally we take for S

$$S = -Et + \vec{p}.\vec{r} \qquad (3.12)$$

where E is given so that Eq.(2.8) is satisfied:

$$E = U + p^2/2m - \hbar^2\kappa^2/2m \qquad (3.13)$$

This solution of the Schrodinger equation is an <u>exact</u> one, but is <u>not unique</u>. This is because <u>condition (3.2) is not necessary although sufficient.</u> In general, da/a may be a function

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*The definition of $\delta^{1/2}$ is indirect. If we differentiate with t $\psi = a \exp(iS/\hbar)$ obtained here, $\partial\delta^{1/2}/\partial t$ is a symbol of which

$$2\delta^{1/2}\frac{\partial \delta^{1/2}}{\partial t} = \partial\delta/\partial t$$

is defined well.

of r; as yet E, (3.13), is an invariant integral of (2.9).

We notice the following three significant characteristics of the solution obtained in the above:

## Stability

Unlike the conventional wave packet, the present one is an exact solution of the Schrodinger equation. Therefore, it is stable in time.

## Particle-likeness

As the magnitude of $\chi$ increases, the solution approaches the representation of a classical material point given by (1.1), as is shown in the appendix. This solution is not an eigenfunction either of energy or of momentum. (The situation is the same also with respect to a conventional wave packet because of its boundary.) However, Ehrenfest-Ruark's theorem (Ref. 5) provides a way to find the gross behavior of this <u>particle</u>.

We define

$$\dot{R} = \frac{\int \psi^* \psi \dot{r} \, d\tau}{\int \psi^* \psi \, d\tau} \qquad (3.14)$$

($d\tau$ : volume element)

Then, according to the theorem,

$$m\ddot{R} = - \frac{\int \psi^* \psi \, \text{grad } U \, d\tau}{\int \psi^* \psi \, d\tau} \qquad (3.15)$$

is obtained from the Schrodinger equation. Since $\psi^* \psi$ is localized narrowly, we may write

$$m\ddot{R} = - \text{grad } U \qquad (3.15)'$$

which has an integral

$$\tfrac{1}{2} m \dot{R}^2 + U = \text{const} \qquad (3.16)$$

Unlike E given by (3.12), this integral does not contain $\hbar^2\kappa^2$.

## Formation of de Broglie wave

In general

$$\psi = \sum_\nu \frac{\alpha_\nu \exp(-\kappa|\vec{r}-\vec{v}t-\vec{\beta}_\nu|)}{|\vec{r}-\vec{v}t-\vec{\beta}_\nu|} \exp\left[i(-Et + m\vec{v}\cdot\vec{r})/\hbar\right] \qquad (3.17)$$

is a solution of the Schrodinger equation for a free particle. Here scalars $\alpha_\nu$ and vectors $\vec{\beta}_\nu$ are arbitrary constants. This is proved by noticing that

$$a = \sum_\nu \frac{\alpha_\nu \exp(-\kappa|\vec{r}-\vec{v}t-\vec{\beta}_\nu|)}{|\vec{r}-\vec{v}t-\vec{\beta}_\nu|} \qquad (3.18)$$

satisfies Eq.(3.2), and hence $a^2$ satisfies Eq.(2.6). If we choose the $\alpha$'s as infinitesimal and let the $\beta$'s fill the entire space, $\psi$ given by (3.17) represents substantially a plane de Broglie wave.

In the above process of forming de Broglie wave, we do not consider any interaction among those many representations of particles. This manifests that the wave is an ensemble representation of single particle in free state. In other words, we may also say that by a de Broglie wave, we represent many similar systems of which each consists of a single particle and among which there is no physical interaction. This statement might sound somehow paradoxical in view of Pauli's principle which prohibits more than one particle to exist in the same state. In the following two sections, we shall clarify this apparent paradox.

## IV. THE LIOUVILLE EQUATION FOR n-PARTICLE SYSTEMS

It is easy to derive the quantum-mechanical Liouville equation from the Schrodinger equation for two particles, named 1 and 2:

$$i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m_1} \Delta_1 \psi + \frac{\hbar^2}{2m_2} \Delta_2 \psi - U \psi = 0 \qquad (4.1)$$

where

$$\Delta_1 = \partial^2/\partial x_1^2 + \partial^2/\partial y_1^2 + \partial^2/\partial z_1^2 \quad , \text{ etc.}$$

$$U = U_{12}(r_1, r_2) + U_{01}(r_1) + U_{02}(r_2) \qquad (4.2)$$

$$\vec{r}_1 = x_1, y_1, z_1 \quad , \text{ etc.}$$

$U_{12}$ is the potential between particle 1 and particle 2; $U_{01}$ is the potential of particle 1 due to external field, and so forth. On substituting in Eq.(4.1)

$$\psi = a \exp(iS/\hbar) \qquad (4.3)$$

and considering the real and imaginary parts of the resultant equation separately, we obtain

$$- a \frac{\partial S}{\partial t} + \frac{\hbar^2}{2m_1}\left[\Delta_1 a - \frac{a}{\hbar^2}(\mathrm{grad}_1 S)^2\right]$$

$$+ \frac{\hbar^2}{2m_2}\left[\Delta_2 a - \frac{a}{\hbar^2}(\mathrm{grad}_2 S)^2\right] - U a = 0 \qquad (4.4)$$

$$\partial a/\partial t + (1/m_1)(\mathrm{grad}_1 a)\cdot(\mathrm{grad}_1 S) + (1/2m_1)\, a\Delta_1 S$$

$$+ (1/m_2)(\mathrm{grad}_2 a)\cdot(\mathrm{grad}_2 S) + (1/2m_2)\, a\Delta_2 S = 0 \qquad (4.5)$$

where

$$\mathrm{grad}_1 = (\partial/\partial x_1, \partial/\partial y_1, \partial/\partial z_1), \text{ etc.}$$

In the same way as in the case of single particle (Ref. 2), we define $\vec{p}_1$ and $\vec{p}_2$ by

$$\vec{p}_1 = \mathrm{grad}_1 S \qquad (4.6)$$
$$\vec{p}_2 = \mathrm{grad}_2 S$$

On regarding t, $\vec{r}_1$, $\vec{r}_2$, $\vec{p}_1$, $\vec{p}_2$ as the independent variables, we obtain for Eq.(4.4)

$$\frac{\partial S}{\partial t} + \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - \frac{\hbar^2}{2m_1}\frac{\Delta_1 a}{a} - \frac{\hbar^2}{2m_2}\frac{\Delta_2 a}{a} + U = 0 \qquad (4.7)$$

and for (4.5)

$$\left\{\frac{\partial}{\partial t} + \frac{\vec{p}_1}{m_1}\cdot\frac{\partial}{\partial \vec{r}_1} + \frac{\vec{p}_2}{m_2}\cdot\frac{\partial}{\partial \vec{r}_2}\right.$$

$$+ \operatorname{grad}_1 \left[ -U + \frac{\hbar^2}{2m_1} \cdot \frac{\Delta_1 a}{a} + \frac{\hbar^2}{2m_2} \cdot \frac{\Delta_2 a}{a} \right] \cdot \frac{\partial}{\partial \vec{p}_1}$$

$$+ \operatorname{grad}_2 \left[ -U + \frac{\hbar^2}{2m_1} \cdot \frac{\Delta_1 a}{a} + \frac{\hbar^2}{2m_2} \cdot \frac{\Delta_2 a}{a} \right] \cdot \frac{\partial}{\partial \vec{p}_2} \Bigg\} a^2 = 0 \qquad (4.8)$$

The same treatment is easily extended to the case of n-particle systems, and the following are obtained:

$$\frac{\partial S}{\partial t} + \sum_{k=1}^{n} \frac{p_k^2}{2m_k} - \sum_{k=1}^{n} \frac{\hbar^2}{2m_k} \frac{\Delta_k a}{a} + U = 0 \qquad (4.9)$$

$$\left[ \frac{\partial}{\partial t} + \sum_{k=1}^{n} \frac{\vec{p}_k}{m_k} \cdot \frac{\partial}{\partial \vec{r}_k} - \sum_{k=1}^{n} \operatorname{grad}_k \breve{U} \cdot \frac{\partial}{\partial p_k} \right] a^2 = 0 \qquad (4.10)$$

where

$$\breve{U} = U - (\hbar^2/2) \sum_{k=1}^{n} (\Delta_k a/a)/m_k \qquad (4.11)$$

$$\vec{p}_k = \operatorname{grad}_k S \qquad (4.12)$$

## V. PAULI'S PRINCIPLE

Earlier, Ref.1, Margenau discussed the limit of validity of the exclusion principle. This pioneering study was made within the framework of conventional quantum mechanics. The present author, some years later, also studied the same matter in a demonstrative manner. Ref. 6. The obvious inadequacy of Pauli's principle, when applied rather axiomatically, manifests the necessity of interpreting conventional solutions of the Schrodinger equation as lacking some information. In this section, Pauli's principle is studied in a somewhat different manner by employing the result of section IV.

We consider a system of two similar particles. We begin our investigation by assuming that the terms containing $h^2$ in Eq.(4.8) are of minor correction.* Then we may think that we ignore them completely in Eq.(4.8) to the first approximation. On substituting a solution thus obtained to the first approximation, in those correction terms, we obtain Eq.(4.8) to the second approximation. After repeating successively similar procedures of approximation, we may obtain a partial differential equation which is a good substitute for Eq.(4.8), and yet is linear and of the first order with respect to $a^2$, because those correction terms are known functions. We may have for

*In section III, we saw that these terms must vanish for a single and free particle. In general, this is not necessary although sufficient for obtaining exact solutions. See section VI.

the characteristic equations of the resultant equation:

$$\frac{d\vec{r}_1}{dt} = \frac{\vec{p}_1}{m_1}$$

$$\frac{d\vec{p}_1}{dt} = -\text{grad}_1(U_{01} + U_{12}) + \text{grad}_1\left(\frac{\hbar^2}{2m_1}\frac{\Delta_1 a}{a} + \frac{\hbar^2}{2m_2}\frac{\Delta_2 a}{a}\right),$$

$$\frac{d\vec{r}_2}{dt} = \frac{\vec{p}_2}{m_2}, \qquad (5.1)$$

$$\frac{dp_2}{dt} = -\text{grad}_2(U_{02} + U_{12}) + \text{grad}_2\left(\frac{\hbar^2}{2m_1}\frac{\Delta_1 a}{a} + \frac{\hbar^2}{2m_2}\frac{\Delta_2 a}{a}\right)$$

These are given in the 12-dimensional phase space. It is possible, to an approximation, to represent them in the 6-dimensional phase space. The representation of one particle is the same as of the other, provided that $m_1 = m_2$:

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} \qquad (5.2)$$

$$\frac{d\vec{p}}{dt} = -\text{grad } U' + \text{grad}\left(\frac{\hbar^2}{2m}\frac{\Delta a}{a}\right)$$

This approximation is made by substituting

$$U' = U_{01} + \langle U_{12}\rangle_{\text{average}}, \text{ for } U_{01} + U_{12} \qquad (5.3)$$

and by assuming that

$$\text{grad}_1\left(\frac{\Delta_2 a}{a}\right) = \text{grad}_2\left(\frac{\Delta_1 a}{a}\right) = 0 \qquad (5.4)$$

These assumptions are permissible, if two particles in the same system are known to be sufficiently remote that, in the space domain where $\Delta_1 a/a$ depends significantly on $r_1$, $\Delta_1 a/a$ is substantially independent of $r_2$, and vice versa. If we rely solely on (5.2), however, there is the danger of making a serious mistake: The trick is that $\Delta a/a$ is independent of the absolute amplitude of a, and hence we tend to think that we may superpose representations of any number of similar particles. Then the solution thus obtained from (5.2) is much different from the solution obtained by solving honestly Eq.(5.1); there, in the 12-dimensional phase space, those terms $U_{12}$, $\Delta_1 a/a$, $\Delta_2 a/a$ prevent the two particles from being superposed in the same local domain of space. In order to substitute (5.2) for (5.1) with no such mistake, we need some additional condition to prevent us from making the mistake. Pauli's principle is the very device to serve for this purpose. Thanks to the principle, we may avoid possible mistakes which will be caused by the inadequacy of (5.2) for the substitute of (5.1).

Being a conventional device such as explained in the above, Pauli's principle cannot be applied mechanically, without causing paradoxical results. (The situation may be usual with respect to any axiom in physics!) Suppose that two similar particles are remote although they are in the <u>same quantum-mechanical state</u>.

In the light of the discussion made in the above, Pauli's principle should not be applied in this case. But, conventional quantum mechanics does not pay attention to this remoteness, since it does not make any distinction between single system and its ensemble. Thus we tend to apply mechanically Pauli's principle and come to a paradox. For example, consider two electrons, of which one is in a hydrogen atom and the other in another hydrogen atom which is remote from the former. If Pauli's principle were applicable, the intensity of any spectrum line observed in a hydrogen gas would be extremely weak, because only one of those numerous electrons is permitted to be in one energy eigen-state at one moment of time.

In general, conventional solutions of the Schrodinger equation lack adequate descriptions of <u>where</u> and <u>when</u>, as usual in ensemble representations. Furthermore, Pauli's principle, made to supplement the inadequacy, cannot alone provide <u>safeguard</u> adequate for preventing our mistake due to the inadequacy of quantum-mechanical descriptions, as demonstrated in the above. From this viewpoint alone, it is necessary, even in the pragmatical spirit, to interpret conventional solutions of the Schrodinger equation as of ensembles. (Since von Neumann's well-known study, it is being accepted that quantum mechanics is a <u>logically consistent</u> system. But this does not mean that quantum mechanics is <u>physically adequate</u>.)

## VI. A PARTICULAR SOLUTION FOR n-PARTICLE SYSTEM

In section III, we obtained an exact solution for one-particle system. The existence of U, potential field, does not bring in any essential difficulty, as long as the condition, $\Delta a/a$ = invariant, is maintained. This condition is not necessary when U exists. Therefore the solution obtained there is expected not to be unique when $U \neq 0$ . The solution is stable, localized in space, and furthermore leads to de Broglie wave when $U = 0$.

It is not difficult to find a similar solution for n-particle system. We write

$$a^2 = \prod_{k=1}^{n} \frac{\exp\left[-2\kappa_k \left| \vec{r}_k - \frac{\vec{p}_k(t)}{m_k} dt \right|\right]}{\left| \vec{r}_k - \frac{\vec{p}_k(t)}{m_k} dt \right|^2} \delta(\vec{p}_k - \vec{p}_k(t)) \tag{6.1}$$

where $p_k(t)$ are solutions of

$$\begin{aligned} \frac{d\vec{p}_k}{dt} &= -\,\mathrm{grad}_k\left(U - \frac{\hbar^2}{2m_k} \sum \Delta_k a/a\right) \\ \frac{d\vec{r}_k}{dt} &= \frac{\vec{p}_k}{m_k} \end{aligned} \tag{6.2}$$

$$U = \sum_k U_{0k} + \sum_{k<j} \sum U_{kj}$$

First easily shown is that

$$\Delta_k\, a/a = \kappa_k^2 \tag{6.3}$$

Hence Eqs.(6.2) are characteristic equations of (4.10). So

$a^2$ given by (6.1) satisfies (4.10). In order to satisfy (4.9) and (4.12), we take

$$S = - Et + \sum_k \vec{p}_k \cdot \vec{r}_k \tag{6.4}$$

Then (4.9) yields

$$-E + \sum \frac{p_k^2}{2m_k} - \sum \frac{\hbar^2}{2m_k} \kappa_k^2 + U = 0 \tag{6.5}$$

E can be invariant only when the p's are chosen so that

$$\frac{p_k^2}{2m_k} + U = \text{invariant}. \tag{6.6}$$

The nontrivial case of (6.1) is realized only when

$$\vec{p}_k = \vec{p}_k(t)$$

and hence, the integral of (6.2)

$$\frac{\vec{p}_k(t)^2}{2m_k} + U = \text{invariant}$$

is the very condition (6.6).

As has been repeated often, this solution is exact, but is not unique. In general, $_k a/a$ may be a function of the r's; as yet, E, (6.5), is an invariant integral of (6.2).

## VII. GENERAL SOLUTION

## (SOLUTION FOR ENSEMBLES)

It is easy to construct general solution (solutions for n-particle ensembles) with the particular solution obtained in section VI. A set of solutions of (6.2)

$$\begin{aligned} &\vec{p}_k(t) \\ &\vec{r}_k(t) \equiv \int \frac{\vec{p}_k(t)}{m_k}\, dt \end{aligned} \qquad (7.1)$$

$$k = 1, 2, \ldots, n$$

have their initial condition

$$\vec{p}_k(0),\ \vec{r}_k(0) \qquad (7.2)$$

contained in them. Then we make, with a given by (6.1),

$$a_g = \int\cdots\int a\, \varphi\left[\vec{p}_1(0), \vec{r}_1(0), \ldots, \vec{p}_n(0), \vec{r}_n(0)\right] \prod_{k=1}^{n} d\vec{p}_k(0)\, d\vec{r}_k(0) \qquad (7.3)$$

where $\varphi$ is an arbitrary function of the intial values (7.2). The function $a_g$ obtained in the above satisfies

$$\frac{\Delta_k a_g}{a_g} = K_k^2 \qquad (7.4)$$

Hence the gradient of it vanishes. In general, we may write

$$a_g^2 = F(\vec{r}_i - \vec{r}_i(t),\ \vec{p}_i - \vec{p}_i(t),\ \ldots\ldots\ldots)$$

Of course, F is a complex function, and unknown in general. But it is obvious that

$$\partial F/\partial t = -\sum_{k=1}^{n}\left(\dot{\vec{r}}_k(t)\cdot\frac{\partial F}{\partial \vec{r}_k} + \dot{\vec{p}}_k(t)\cdot\frac{\partial F}{\partial \vec{p}_k}\right)$$

Hence $a_g^2$ satisfies the Liouville equation (4.10) under condition (7.4).

For S, we take

$$S = -E(t) + \sum \vec{p}_k\cdot\vec{r}_k \tag{7.5}$$

Then (4.9) yields

$$-\dot{E}(t) + \sum\frac{p_k^2}{2m_k} - \sum\frac{\hbar^2}{2m_k}\kappa_k^2 + U = 0 \tag{7.6}$$

Unlike the case of (6.6), condition (7.6) is not always satisfied by those independent variables t, $\vec{p}_k$ , $\vec{r}_k$. Note that U is a function of the r's. Condition (7.6) imposes a restriction on those independent variables.

## VIII. DISCUSSION AND CONCLUSION

Those solutions of the Schrodinger equation obtained in this report are exact, with two restrictions:

a) $\Delta a/a$ = invariant.

b) Solutions of Newton's equations of motion are given: Because of condition a), the characteristic equations of the quantum-mechanical Liouville equation turn out to be of the relevant classical Liouville equqtion. That is why condition b) is necessary.

Condition a) is surely necessary when a particle is completely free, and the de Broglie wave is composed by superposing many similar solutions obtained for single particle. But, when a particle is in a force field, it is unlikely that condition a) is necessary in general. Nevertheless, assuming condition a) does not lead to any inconsistency of the solution; this is a remarkable situation. Therefore, it may be reasonable to assume condition a) to be valid when force field is not extremely strong. Accordingly, except for lowest energy levels, conventional energy eigen-solutions may be special cases of the general solutions obtained in section VII. (With a particular reason, the one-dimensional oscillator is an exception.) In summary :

1. There is a wavelet, as an exact solution of the Schrodinger equation, which seems to represent a particle in free state.

2. The de Broglie wave is constructed with similar wavelets.

3. The wavelet approaches the known $\delta$-function representation of a classical-mechanical particle in the phase space, as a parameter approaches its limit value.

4. The quantum-mechanical Liouville equation for n-particle system is obtained.

5. Pauli's principle, with its merit and paradox, is explained as based on the Liouville equation for n-particle system.

6. An exact solution for single n-particle system is obtained, if the relevant solutions of Newton's equations are given.

7. In the same sense, an exact ensemble solution of n-particle systems is obtained.

8. Relevant solutions for the Dirac equation are expected to exist.

In view of these characteristics, solutions obtained in this report undoubtedly promise the possibility of kinetic theory of quantum-mechanical systems, provided that emission-absorption processes are not significant in those systems. In order to take into account emission-absorption processes, consideration of solutions of the Schrodinger equation is not sufficient; similar solutions of the Dirac equation are necessary.

## APPENDIX

## Connection Between $\delta$-Function and $\underline{a}$ or $\underline{a}^2$ Given by (3.6)

We define

$$A(\kappa, \epsilon) = \iiint \frac{\exp(-\kappa\sqrt{x^2+ y^2+ z^2})}{\sqrt{x^2+ y^2+ z^2}}\, dxdydz \tag{A.1}$$

where the domain of integration should be limited by

$$x^2 + y^2 + z^2 \geq \epsilon^2 \tag{A.2}$$

so that $A(\kappa, \epsilon)$ does not diverge. As $\kappa$ increases, $\epsilon$ may be smaller. Then we define

$$D(x,y,z, \kappa, \epsilon) = \frac{\exp(-\kappa\sqrt{x^2+ y^2+ z^2})}{A(\kappa,\epsilon)\sqrt{x^2+ y^2+ z^2}} \tag{A.3}$$

in the same domain of x,y,z, as (A.2). Of course, we have

$$\iiint D(x,y,z,\kappa,\epsilon)dxdydz = 1 \tag{A.4}$$

However, if $\kappa$ is sufficiently large, (A.4) will be satisfied by taking for the domain of integration

$$R^2 \geq x^2+ y^2+ z^2 \geq \epsilon^2 \tag{A.5}$$

instead of (A.2). This is becsuse, for large $\kappa$ , contribution to the integral (A.4) is made only by $x^2+ y^2+ z^2$ of small values.

As $\kappa$ increases, the permissible limits of R and of $\epsilon$ decrease. In other words, function D is more localized near $x = y = z = 0$, as $\kappa$ increases. As yet, it satisfies (A.4). This is the very characteristic of $\delta(x)\delta(y)\delta(z)$.

It is noted that $a^2$ has the same characteristic at the limit $\kappa \to \infty$.

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13. ABSTRACT

The quantum-mechanical Liouville equation is more restrictive and hence more informative than the Schrodinger equation, because the former already contains the definition of independent variable $\vec{p}$, momentum in a special case. In this sense, the quantum-mechanical Liouville equation is more definitive as the description of a physical law, and is shown to be invariant under the Galilean transformation. By taking advantage of this convenience, we obtain a particular solution of the Schrodinger equation for n-particle system. This solution is localized in the phase space and stable in time, and seems to represent an n-particle system as single system. The de Broglie wave is constructed by superposing a number of similar particular solutions for single-particle systems. Similarly, general solution is constructed for n-particle systems. For justification of its application to kinetic theory, Pauli's principle is analyzed and interpreted anew. The present solution promises the possibility of rational methods of kinetic theory of quantum-mechanical systems, as analogous to methods of classical kinetic theory.

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